Modern Computational Tools for Reactor Safety

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Overview of Thermal Hydraulic and CFD capabilities at LANL

- Historical knowledge of both the TRAC and RELAP codes
- 3-D chemically reacting flow for combustion: **KIVA**
- Two-phase 3-D CFD capability : **CFDLIB**
- 3-D multi-physics (Rad/Hydro) massively parallel simulations: **CHAD**
- Modern software engineering **: CartaBlanca**
- Follow-on generation Rad/Hydro codes : **Marmot**
- Liquid metal (melting/solidification) modeling : **Telluride**
- Modern methods : Jacobian-free Newton-Krylov (**JFNK**), physics-based preconditioning, etc
- Extensive experience with parallel code development on current computing platforms, including processor communication, debugging, viz, etc

Historical Knowledge of two-phase flow modeling

- The semi-implicit method employed by many thermal hydraulic codes was developed at LANL in T-Division
- Initial work on the TRAC code was done at LANL in T-Division
- Personal currently in T-Division have also worked at INL and the NRC on RELAP
- LANL maintains collaboration with other labs, universities, and industry.

KIVA capabilities (20 years old)

- Two-phase droplet model (Eulerian gas, Lagrangian droplet)
  - Collision
  - Breakup
  - Phase change
  - Wall droplet interactions
- Moving boundaries and mesh
- Chemical reactions
- Unstructured mesh
- Parallel

CFDLIB capabilities (15 years old)

- 3D Two-phase flow with mass transfer
- Easily modified source code that is readily available to government contractors
- Has already been used to develop closure & sub-grid models for 1-D system codes
- Parallel
- Unstructured grids
- Fluid/structure interactions

CHAD capabilities (8 years old)

- 3-D radiation diffusion model
- 3-D Eulerian two-phase flow
- Lagrangian particle two-phase flow model
- Moving molten material model
- Multi-material turbulence models
- Massively parallel - tested on modern platforms
- Arbitrary Lagrangian Eulerian (ALE)
- Fully implicit CFD - accurate with large time steps

CartaBlanca capabilities (5 years old)

- Multi-physics multi-phase simulation code
- Based on modern multiphase flow theories
- Advanced computational methods
- Written in the object-oriented computer language Java
- Fluid dynamics
- Heat/mass transfer
- Chemical reactions
- Mechanical stresses and thermal stresses
- Fluid structure interactions

Modern Methods

- Jacobian-free Newton-Krylov (JFNK)
  - Solve the coupled nonlinear system of equations in a single solve
  - Improves accuracy by eliminating the errors associated with linearizations and operator splitting
  - Easily made second order accurate
  - Easily parallelizable
- Physics-Based Preconditioning
  - Use old solution algorithms (such as semi-implicit) as a preconditioner
  - Provides a hybrid algorithm which is fast (semi-implicit) and accurate (JFNK)

Summary of LANL Capabilities

- Historical knowledge of existing tools and many of the methods employed in the existing tools were developed here.
- Arguably the birth place of Computational Fluid Dynamics (CFD) and it continues to be a leader in CFD today
- A strong methods development capability.
- Knowledge of accurate modern solution methods, modern software engineering, and availability of source code makes LANL a logical partner for reactor safety simulation work.
- Extensive massively parallel experience gained from the ASC project